SOZLab

Linux GUI + CLI for solvent occupancy zone analysis

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SOZLab Tutorial

What SOZLab does

SOZLab is a Linux GUI + CLI for solvent occupancy zone (SOZ) analysis of MD trajectories. It evaluates, per frame, which solvent residues satisfy a user-defined logic tree around one or more seed selections and reports occupancy, entry/exit events, residence statistics, plots, and extractable frame sets.

Operational definition of a SOZ

A SOZ is the set of solvent residues that satisfy a logic tree in a given frame. The evaluated set is residue-based (resindices/resids), not atoms. All occupancy counts and events refer to solvent residues, which avoids atom-count bias for multi-atom solvents.

Per-frame metrics (definitions)

1. **frame**: zero-based trajectory frame index after applying **analysis.frame_start**, **analysis.frame_stop**, and **analysis.stride**.
1. **time**: **ts.time** from MDAnalysis for the frame. Values are written to CSV as-is.
1. **n_solvent**: integer count of solvent residues in the SOZ for that frame.
1. **entries**: number of solvent residues that appear relative to the previous sampled frame.
1. **exits**: number of solvent residues that disappear relative to the previous sampled frame.

Stride effects (critical)

Entries and exits are computed between sampled frames. If **analysis.stride** is large, short-lived events can be missed and entry/exit counts only reflect changes between sampled frames.

Units and time bases

1. Length cutoffs accept **unit: "A"** or **unit: "nm"**. Internally, SOZLab converts to angstroms (1 nm = 10 A).
1. Time comes directly from MDAnalysis. The GUI divides **time** by 1000 and labels it in ns (assumes ps input). If your trajectory time units are not ps, confirm the unit before interpreting plots.
1. GROMACS conventions use nm for length and ps for time. Always validate your expectations when switching between toolchains.

Quick start

GUI quick start (sample project)

1) Launch: **sozlab-gui**. 2) Click **Load** (header bar) and open **examples/sample_project.json**. 3) In the left drawer, review **Inputs**, **Analysis Window**, and **Output Settings**. 4) Click **Run**. The status bar shows progress and a log path. 5) Use the stepper tabs: **Project**, **Define**, **QC**, **Explore**, **Export**. 6) In **Explore**, inspect the Timeline and plots. Use **Export Data** or **Export Report** when ready.

CLI quick start (sample project)

```
sozlab-cli run --project examples/sample_project.json --output out --progress --report
```

Validation (fast sanity check):

```
sozlab-cli validate --project examples/sample_project.json --max-frames 200
```

Extraction example:

```
sozlab-cli extract --project examples/sample_project.json --soz shell_only --rule
"n_solvent>=1" --min-run 5 --gap 1 --out out/extracted
```

Example projects

1. **examples/sample_project.json**: minimal example.
1. **examples/gromacs_template_project.json**: GROMACS-oriented template.
1. **examples/soz_configs/**: individual SOZ definitions for Advanced JSON.

CLI reference (current flags)

Run

```
sozlab-cli run --project PROJECT [--output OUTPUT] [--stride STRIDE] [--start START]
[--stop STOP] [--no-ids] [--no-per-frame] [--progress] [--report]
```

1. **--project**: project JSON file (required).
1. **--output**: output directory for results and logs.
1. **--stride**: frame stride override.
1. **--start**: start frame index.
1. **--stop**: stop frame index (exclusive).
1. **--no-ids**: disable per-frame solvent IDs.
1. **--no-per-frame**: disable per-frame table export.
1. **--progress**: show progress bar in terminal.
1. **--report**: generate report after analysis.

Validate

```
sozlab-cli validate --project PROJECT [--max-frames MAX_FRAMES]
```

1. **--project**: project JSON file (required).
1. **--max-frames**: maximum frames to validate (default 200).

Extract

```
sozlab-cli extract --project PROJECT [--soz SOZ] [--rule RULE] [--min-run MIN_RUN] [--gap
GAP] [--out OUT] [--format FORMAT] [--prefix PREFIX] [--output OUTPUT]
```

1. **--project**: project JSON file (required).
1. **--soz**: SOZ name to filter.
1. **--rule**: rule string (e.g., **n_solvent>=1**).
1. **--min-run**: minimum consecutive frames.
1. **--gap**: gap tolerance to merge runs.

1. **--out**: extraction output directory.
1. **--format**: trajectory format (default **xtc**).
1. **--prefix**: output filename prefix (default **extracted**).
1. **--output**: override output dir for logs only.

Output directory behavior

1. **outputs.output_dir** is the base directory for logs and exported results.
1. GUI **Output Settings** edits **outputs.output_dir**. Export Data/Report prompts for a directory and updates this value.
1. CLI **run --output OUT** overrides **outputs.output_dir** for that run.
1. CLI **extract --output OUT** overrides only the log directory; **extract --out OUT_EXTRACT** controls extraction outputs.

UI overview (layout and navigation)

Header bar

1. Stepper: **Project**, **Define**, **QC**, **Explore**, **Export** (switches main pages).
1. Actions: **Load**, **Save**, **New SOZ**, **Quick**, **Run**, **Cancel**, **Export Data**, **Export Report**.
1. Toggles: **Console** (diagnostics console), **Drawer** (left panel), **Inspector** (right panel).
1. UI controls: **Theme** (Light/Dark), **Scale**, **Presentation** (larger UI, hides drawers).
1. Shortcuts: see the Appendix.
1. Command palette (**Ctrl+K**) opens a searchable list of common actions.

Action behavior:

1. **Load** opens a project JSON/YAML file.
1. **Save** writes the current project to JSON/YAML (prompts on first save).
1. **New SOZ** applies the current Wizard definition to the project.
1. **Quick** sets a coarse stride based on **analysis.preview_frames** and runs a fast preview.
1. **Run** enforces Project Doctor checks before analysis.
1. **Cancel** stops an in-progress run.

Main layout

1. Left drawer: project settings, output settings, Project Doctor, defined SOZ list.
1. Center page: content for the selected stepper page.
1. Right inspector (optional): context-sensitive status for the current page.

1. Bottom console (optional): recent log lines and quick refresh.
1. Status bar: run status messages and progress bar.

Inspector contents (when enabled):

1. Project: Provenance Stamp with copy button.
1. Define: live selection status tips.
1. QC: QC status summary.
1. Explore: active SOZ, metric, and time window.
1. Export: extraction status hints.

Project step (inputs and run configuration)

If no project is loaded, **Run** or **Quick** will prompt for topology and optional trajectory, then create a default project in memory.

Inputs (left drawer)

1. **Topology**: label shows current file; **Change** opens a file dialog.
1. **Trajectory**: label shows current file; **Change** and **Clear** manage it.
1. **Metadata**: summary line (SOZ count, selection count, stride, frames if available).

Analysis Window (left drawer)

1. **Frame start**: integer start frame index.
1. **Frame stop**: integer stop frame index; use **End** to include full trajectory.
1. **Stride**: sampling stride (integer >= 1).

Output Settings (left drawer)

1. **Output dir**: base directory for analysis outputs and logs.
1. **Report format**: **html** or **md**.
1. **Write per-frame CSV**: controls whether **per_frame.csv** is written.
1. **Write parquet**: writes **.parquet** alongside CSV (requires **pyarrow**).

Project Doctor (left drawer)

1. **Run Project Doctor**: preflight checks on inputs, selections, solvent, probe, units, and PBC.
1. **PBC Helper**: shows recommended **gmx trjconv** commands for preprocessing.
1. Selection table: lists selection labels, counts, uniqueness requirements, and suggestions (columns: Selection label, Count, Require unique match, Expect count, Selection, Suggestions).

Defined SOZs (left drawer)

1. List of SOZ definitions currently in the project file.

Project page (center)

1. **Project Summary**: topology/trajectory details and PBC status.
1. **Run Summary**: summarized results after analysis; **Show raw JSON** reveals raw summary.

Define step (SOZ builder tabs)

Wizard tab (main builder)

Fields and controls:

1. **SOZ name**: name for the SOZ definition.
1. **Solvent label**: display label only (does not change selection logic).
1. **Solvent resnames**: comma-separated residue names used to identify solvent molecules.
1. **Probe selection**: MDAnalysis selection applied within solvent residues.
1. **Probe position**: **atom**, **com**, or **cog**.
1. **Include ions** + **Ion resnames**: optional ion residues included as solvent.
1. **Selection A** + **Selection A unique match**.
1. **Shell cutoffs (A)**: comma-separated values in angstroms.
1. **SOZ probe mode**: **probe**, **atom**, **com**, **cog**, or **all**.
1. **Selection B (optional)** + **Selection B unique match**.
1. **Selection B cutoff (A)**.
1. **Selection B combine**: **AND** or **OR**.
1. **Explain my SOZ**: a readable summary of the current wizard definition.
1. **Preview**: evaluates the SOZ for frame 0 (requires inputs).

Notes:

1. The Wizard uses angstrom inputs only. To use **unit: "nm"**, edit the SOZ JSON in **Advanced**.
1. **Probe position = com** requires atom masses in the topology; otherwise, use **cog**.
1. The Wizard stores the probe in **solvent.probe** and keeps legacy **water_oxygen_names** in sync.

Selection match preview (Wizard)

1. **Live**: update when inputs change.
1. **Use trajectory**: include trajectory frames, not just topology.
1. **Max rows**: limit output rows.

1. **Preview**: Selection A or Selection B.
1. Status lines show match counts and suggestions (columns: Atom index, Atom name, Residue name, Residue number, Segment ID, Chain ID, Molecule type).

Selection Builder tab

Builds MDAnalysis selection strings:

1. **Scope**: all atoms, protein, backbone, sidechain, nucleic.
1. **Resname**, **Resid/resnum**, **Atom name**, **Segid**, **ChainID**.
1. **Build** generates the selection string.
1. **Use as Selection A/B** sends to Wizard.
1. **Send to Tester** pushes to Selection Tester.

Bridges tab

Defines solvent bridges between two selections.

1. Table columns: **name**, **selection_a**, **selection_b**, **cutoff_a**, **cutoff_b**, **unit**, **probe_mode**.
1. **Add Bridge**, **Remove Selected**.
1. Each bridge produces **bridge_<name>/** outputs.

Residue Hydration tab

Counts residue contacts with solvent in the SOZ.

1. Table columns: **name**, **residue_selection**, **cutoff**, **unit**, **probe_mode**, **soz_name**.
1. **hydration_freq** is the fraction of frames where the residue contacts the solvent set.
1. If **soz_name** is empty, the first SOZ is used.

Advanced tab

1. Paste a SOZ JSON definition and click **Apply JSON to SOZ list**.
1. Use this for multi-branch trees, non-A units, or advanced probe modes.

Selection Tester tab

1. **Test Selection**: evaluates a selection string.
1. **Test Probe**: evaluates the current solvent probe selection.
1. **Max rows** and **Load trajectory** control sampling.
1. Results list atom/residue identifiers and suggestions (columns: index, resname, resid, resnum, segid, chainID, moltype, name).

QC step

QC Summary page

1. **QC Summary**: a readable summary of preflight and run-time warnings.
1. **Show raw QC JSON**: shows raw QC payload.
1. **Diagnostics** tab: log viewer (same controls as the Logs tab).

Diagnostics and logs

1. **Log path**, **Refresh**, **Open Log**, **Copy Errors**.
1. Filters: Level (All/INFO/WARNING/ERROR), search box, **Collapse tracebacks**.

Explore step (interactive analysis)

Timeline top area (tabbed)

The top plot region is tabbed: **Timeline** and **Entry/Exit** share the same plot area.

Timeline tab (Occupancy Timeline)

Controls:

1. **SOZ** selector.
1. **Metric** and **Secondary** (secondary plots on right axis).
1. **Smooth** + **Window** (rolling mean in frames).
1. Display toggles: **Overlay all SOZs**, **Step plot**, **Markers**, **Clamp y>=0**, **Mean line**, **Median line**, **Shade occupancy** (threshold), **Brush time window**.
1. **Clear brush** resets the time window.
1. Actions: **Save Plot**, **Copy** (clipboard), **Export** (file dialog).
1. **Compute Timeline Statistics** calculates summary metrics (mean, median, entries/exits, residence stats).

Axes:

1. X-axis: time in ns (GUI divides **time** by 1000).
1. Y-axis: selected metric (count or fraction depending on metric).

Metric meanings:

1. **n_solvent**, **entries**, **exits** are counts per frame.
1. **occupancy_fraction** is 0/1 per frame (1 when **n_solvent>0**).

Brush behavior:

1. When enabled, the brush time window filters Histogram, Heatmap, Event Raster, and tables.

Entry/Exit tab (Entry/Exit Rate)

Controls:

1. **Entry/Exit mode**: Events per frame, Rate (events/ns), Cumulative events.
1. **Normalize**: per ns, per 100 frames, or none (disabled for Rate/Cumulative).
1. **Bin (ns)**: aggregates entries/exits into time bins (0 disables binning).
1. **Split axes** and **Exits negative** adjust visualization.
1. Actions: **Save Plot**, **Export Entry/Exit CSV**.

Axes:

1. X-axis: time in ns.
1. Y-axis: events per frame, events/ns, or cumulative events depending on mode.

Note: If **entries**/**exits** are missing, the GUI derives them from changes in **n_solvent** and warns in the status bar.

Plots tab

Contains three plots (tabs): Histogram, Matrix / Heatmap, Event Raster.

Histogram

Controls: **Histogram metric**, **Bins**, **Normalize**, **Log Y**, **Split zeros**, **Plot Histogram**, **Save Plot**, **Copy**.

Axes:

1. X-axis: selected metric (count or time in ns if **time**).
1. Y-axis: frame count or fraction of frames if normalized.

Notes:

1. Red line = mean; green line = median.
1. **Split zeros** separates zero vs non-zero frames and computes mean/median on the non-zero subset.

When this plot is misleading:

1. If most frames are zero occupancy, the histogram hides when occupancy occurs. Use Timeline or Event Raster.
1. Large stride compresses transient events and can bias the distribution.

Matrix / Heatmap

Controls: **Matrix source**, **Top solvents**, **Min occ %**.

Modes:

1. **Solvent occupancy (top N)**: binary presence matrix for the top N solvents by occupancy.
1. X-axis: time in ns.
1. Y-axis: solvent rank (row 0 = most occupied).
1. Color: 1 = present, 0 = absent.
1. **Residue hydration**: heatmap of **hydration_freq** per residue (requires residue hydration config).

Note: Heatmap requires per-frame solvent IDs (**analysis.store_ids=true**).

Event Raster

Controls: **Event stride**, **Segments**, **Min duration**.

Axes:

1. X-axis: time in ns.
1. Y-axis: solvent rank (same ordering as the heatmap).

Interpretation:

1. Points show occupancy events; **Segments** shows continuous occupancy spans.

When this plot is misleading:

1. High stride can hide short events or merge nearby events.
1. Small Top N can hide rare but important solvents.

Tables tab

1. **Filter**: text filter for row filtering.
1. Tabs: **Per Frame**, **Per Solvent**.
1. Tables are sortable; filtering applies to the active table.

Export step (data, report, extraction)

Export Data

1. Writes **metadata.json**, **soz_<name>/**, **bridge_<name>/**, and **hydration_<name>/** outputs to disk.
1. Uses the Output Settings directory unless overridden in the export dialog.

Export Report

1. Generates **report/report.md** and plots; **report/report.html** if **report_format=html**.
1. The Report panel shows the output path and copies it to the clipboard after export.

Extract tab (GUI)

Modes:

1. **Threshold**: rule-based filtering with operator and threshold.
1. **Percentile**: selects frames at/above a percentile of the metric distribution.
1. **Top N frames**: selects the top N frames by metric (ties may add frames).

Controls:

1. **SOZ**, **Metric**, **Operator**, **Threshold**, **Percentile**, **Top N frames**.
1. **Min run length** and **Gap tolerance** (disabled for Top N mode).
1. **Format**: currently **xtc**.
1. **Output directory** and **Use Output Settings directory** toggle.
1. **Preview** computes the rule and preview table; **Extract** writes outputs.

Outputs:

1. **<prefix>.xtc**: extracted trajectory.
1. **<prefix>_ref.pdb**: reference structure (first selected frame).
1. **<prefix>_frames.csv**: manifest (frame, time, n_solvent, optional solvent_ids hash).
1. **<prefix>_params.json**: extraction parameters.

Plot export and PowerPoint guidance

Export formats

Save Plot offers: PNG, SVG, EMF, PDF, CSV.

1. **PNG**: raster image.
1. **SVG**: vector (sanitized for PowerPoint edits).
1. **EMF**: Office-friendly vector, best with Inkscape installed.
1. **PDF**: vector, best with Inkscape installed.
1. **CSV**: plot data (timeline, histogram, heatmap, event raster, entry/exit).

PowerPoint tips

1. SVG: Insert > Pictures, then Ungroup (or Convert to Shape). If Ungroup fails, try a cut/paste cycle.
1. EMF: Insert > Pictures, then Group > Ungroup (accept conversion prompt).
1. For best fidelity, install Inkscape so SVG->EMF/PDF conversions use **--export-area-drawing**.

Plot CSV outputs (for reproducibility)

1. Timeline CSV: **time_ns**, metric column, optional secondary metric; includes **soz** when overlay is enabled.
1. Entry/Exit CSV: **time_ns**, **count**, **delta**, **entries**, **exits**, **entry_rate**, **exit_rate** (entries/exits follow current normalization/binning).
1. Histogram CSV: **bin_left**, **bin_right**, **bin_center**, **count** (fraction if normalized).
1. Heatmap CSV: **solvent_id** plus time columns (solvent occupancy) or hydration table columns for residue hydration.
1. Event Raster CSV: points (**solvent_id**, **row**, **frame**, **time_ns**) or segments (**solvent_id**, **row**, **start_frame**, **end_frame**, **start_ns**, **end_ns**, **duration_frames**).

Project JSON schema (current)

Minimal skeleton

```
{
  "version": "1.0",
  "inputs": {
    "topology": "path/to/topol.tpr",
    "trajectory": "path/to/traj.xtc"
  },
  "solvent": {
    "solvent_label": "Water",
    "water_resnames": ["SOL", "WAT", "TIP3", "HOH"],
    "water_oxygen_names": ["O", "OW", "OH2"],
    "water_hydrogen_names": ["H1", "H2", "HW1", "HW2"],
    "probe": {
      "selection": "name O OW OH2",
      "position": "atom"
    },
    "ion_resnames": ["NA", "CL"],
    "include_ions": false
  },
  "selections": {
    "selection_a": {
      "label": "selection_a",
      "selection": "protein and resid 10 and name CA",
      "require_unique": true
    }
  },
  "sozs": [],
  "analysis": {
    "frame_start": 0,
    "frame_stop": null,
    "stride": 1,
    "gap_tolerance": 1,
    "store_ids": true,
    "store_min_distances": true,
    "preview_frames": 200
  },
  "outputs": {
    "output_dir": "results",
    "write_per_frame": true,
    "write_parquet": false,
    "report_format": "md"
  },
  "extraction": {
    "rule": "n_solvent>=1",
    "min_run_length": 1,
    "gap_tolerance": 0,
    "output_format": "xtc",
    "output_dir": "results/extracted"
  },
  "bridges": [],
  "residue_hydration": []
}
```

Selections

1 Use **selections** (preferred) or legacy **seeds**.

1. Each selection supports either a full **selection** string or structured fields (**resid**, **resname**, **atomname**, **segid**, **chain**, **atom_indices**, **pdb_serials**).
1. **require_unique** enforces a single-atom match.
1. Bridges also accept legacy **seed_a** and **seed_b** keys.

SOZ logic tree

1. Node types: **distance**, **shell**, **and**, **or**, **not**.
1. Use **selection_label** in node params (legacy **seed_label** or **seed** are normalized).
1. Cutoffs accept **unit: "A"** or **unit: "nm"**.
1. Probe mode key is **probe_mode** (legacy **atom_mode** also accepted).

Allowed probe modes:

1. **probe**: use **solvent.probe.position**.
1. **atom**: use probe atoms directly.
1. **com**: center of mass of probe atoms per solvent residue (requires masses).
1. **cog**: center of geometry of probe atoms per residue.
1. **all**: all atoms in solvent residues.
1. Legacy **O** is treated as **atom**.

Solvent configuration

1. **water_resnames**: residue names that identify solvent molecules (UI shows "Solvent resnames").
1. Legacy alias: **solvent_resnames** is accepted in project JSON.
1. **probe.selection**: MDAnalysis selection for probe atoms within solvent residues.
1. **probe.position**: **atom**, **com**, or **cog** (global default).
1. **water_oxygen_names** and **water_hydrogen_names** are legacy fields kept for compatibility.
1. **solvent_label** is a display label only; set it to the actual solvent name for clarity (e.g., Methanol, DMSO).

Bridges

Each bridge uses two selections and two cutoffs.

1. **selection_a**, **selection_b**, **cutoff_a**, **cutoff_b**, **unit**, **probe_mode**.

Residue hydration

1. **residue_selection**: residues to score for hydration.
1. **cutoff**, **unit**, **probe_mode**.
1. **soz_name**: optional SOZ to use; default is the first SOZ.

Outputs and file map

Output map

Path	Meaning
metadata.json	Project snapshot, warnings, QC summary.
soz_<name>/per_frame.csv	Per-frame time series and events.
soz_<name>/per_solvent.csv	Per-solvent residence and occupancy summary.
soz_<name>/summary.json	Aggregated SOZ summary metrics.
soz_<name>/min_distance_traces.csv	Min distance traces per selection (if enabled).
bridge_<name>/per_frame.csv	Bridge-specific per-frame table.
bridge_<name>/per_solvent.csv	Bridge-specific per-solvent table.
hydration_<name>/hydration_table.csv	Residue hydration table.
report/report.md	Report markdown with figures.
report/report.html	Report HTML (if report_format=html).

per_frame.csv columns

1. **frame**, **time**, **n_solvent**, **entries**, **exits**.
1. **solvent_ids** (semicolon-delimited **resname:resid:segid**) if **analysis.store_ids=true**.
1. Optional min-distance columns (one per selection) if **analysis.store_min_distances=true**.

per_solvent.csv columns

1. **solvent_id**, **resindex**, **resname**, **resid**, **segid**.
1. **frames_present**, **occupancy_pct**, **entries**.
1. **mean_res_time_cont**, **median_res_time_cont**.
1. **mean_res_time_inter**, **median_res_time_inter**.

summary.json key fields

1. **n_frames**, **frame_stride**, **dt**, **time_unit**.
1. **occupancy_fraction**: fraction of sampled frames with **n_solvent > 0**.
1. **mean_n_solvent**, **median_n_solvent**, **max_n_solvent**.
1. **n_solvent_hist**, **entry_rate**, **exit_rate**.

Extraction (GUI + CLI)

Rule format

Rules are simple comparisons against per-frame metrics:

1. **n_solvent>=1**
1. **entries>=2**

1. **occupancy_fraction==1**

occupancy_fraction is computed per frame as 1 if **n_solvent>0**, else 0.

CLI extraction example

```
sozlab-cli extract \
  --project /path/to/project.json \
  --soz shell_only \
  --rule "n_solvent>=2" \
  --min-run 10 \
  --gap 2 \
  --out /path/to/extracted
```

Validation of extraction

1) Confirm **<prefix>_frames.csv** matches the expected number of frames. 2) Cross-check against **per_frame.csv** for the same SOZ. 3) Load **<prefix>_ref.pdb** and **<prefix>.xtc** in a viewer for spot checks.

Reproducibility and QC

1. Keep the project JSON and **metadata.json** for each run.
1. Record **analysis.frame_start**, **analysis.frame_stop**, **analysis.stride**, and **analysis.gap_tolerance**.
1. Use **sozlab-cli validate --project ... --max-frames 200** to compare fast vs slow evaluation.
1. Store preprocessing context in **inputs.processed_trajectory** and **inputs.preprocessing_notes**.

Troubleshooting (Symptom -> Confirm -> Fix)

Selection resolves to 0 atoms

Confirm: Selection Tester shows 0 hits. Fix: Verify resname/resid, add segid/chainID, or adjust selection scope.

Selection not unique but require_unique is checked

Confirm: Selection Tester shows multiple hits. Fix: Add segid/chainID/resid or disable require_unique.

Solvent resnames do not match any residues

Confirm: Project Doctor reports no solvent matches. Fix: Update **solvent.water_resnames** to match your topology.

Probe selection resolves to 0 atoms or misses residues

Confirm: Selection Tester -> Test Probe shows 0 hits or missing residues. Fix: Update **solvent.probe.selection** and **solvent.probe.position**.

Probe position com fails

Confirm: Error mentions missing masses. Fix: Add atom masses in the topology or use **probe.position: "cog"**.

Logic tree yields zero occupancy

Confirm: **per_frame.csv** has **n_solvent=0** for all frames. Fix: Check cutoffs and selection labels; use the Wizard Preview to test frame 0.

Heatmap/Event Raster says "No solvent IDs available"

Confirm: **per_frame.csv** lacks **solvent_ids**. Fix: Set **analysis.store_ids=true** (CLI: omit **--no-ids**).

Entry/Exit plot is flat

Confirm: **entries** and **exits** are zero or derived from **n_solvent**. Fix: Reduce stride, re-run with per-frame output enabled.

Per-frame tables are too large

Confirm: Disk usage is large or export is slow. Fix: Set **outputs.write_per_frame=false** (CLI: **--no-per-frame**).

Output directory not writable

Confirm: Logs show write errors. Fix: Update Output Settings or pass **--output** for CLI runs.

CLI command not found

Confirm: **sozlab-cli --help** fails. Fix: Activate the **sozlab** environment or run the installed script from your env.

SVG/EMF not editable in PowerPoint

Confirm: SVG opens as an icon or EMF is corrupted. Fix: Export again with Inkscape installed; use the PowerPoint tips above.

Appendix: keyboard shortcuts

1. **Ctrl+O**: Load project
1. **Ctrl+S**: Save project
1. **Ctrl+R**: Run analysis
1. **Ctrl+Shift+R**: Export report
1. **Ctrl+E**: Export data
1. **Ctrl+P**: Toggle presentation mode
1. **Ctrl+K**: Command palette

1. **Ctrl++** or **Ctrl+=**: Increase scale
1. **Ctrl+-**: Decrease scale
1. **Ctrl+0**: Reset scale
1. **Ctrl+Q**: Quit
1. **Ctrl+Mouse Wheel**: Adjust scale